Superconductivity Induced by Negative Centers

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Abstract

We study the effect of random dilution of attraction centers on electron pairing in a generalization of the negative U Hubbard model where the interaction U_i, defined on the two dimensional lattice, can be $-|U|$ and 0 with probability c and $1-c$ depending on the lattice site i. Using the determinant quantum Monte Carlo approach, we find the critical concentration c_0 of negative centers which leads to superconductivity, and show how the evolution of the local density on the two types of sites lends insight into the formation of global phase coherence.

Key words: disorder, doping, fluctuations
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1 Introduction

The behavior of High Temperature Superconductors (HTS) is characterized by a strong dependence on doping. For example, changing the Sr concentration in $La_{2-x}Sr_xCuO_4$, or the O concentration in $YBa_2Cu_3O_{6+\delta}$ tunes these materials from antiferromagnetic insulators, to spin glasses, and finally to superconductors. The short coherence length and relatively low superfluid density in the underdoped region emphasize the existence of phase fluctuations and enhance

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the competition between superconductivity and other long range order phases [1,2]. In such systems, where different ground states emerge as the particle density is tuned, it is often important to explore the possibility inhomogeneous mixtures of phases; for example, 'antiferromagnetic' and 'superconducting', at commensurate and incommensurate filling. Indeed, there has already been considerable study of whether the doped holes are uniformly distributed or whether they accumulate preferentially in two-dimensional phase separated regions[3] or in one-dimensional stripes[4].

There have been many direct studies of doping dependent transitions in correlated electron Hamiltonians like the repulsive Hubbard model, which provide microscopic models of HTS[5,4]. These are numerically challenging since they attempt to understand the origin of HTS at the same time as addressing additional subtle issues like inhomogeneous phases. A more simple, if somewhat less fundamental, way in which related questions can be addressed is to consider models, like the $-U$ Hubbard Hamiltonian, which have an attractive interaction 'built in'. This separates out the problem of how superconducting pairs form in disordered, short coherence length systems in which the particle density is fixed but the interactions are diluted, from the complexities of the origins of the attractive interaction. The key underlying question is how superconductivity spreads through a system as the local attraction between charge carriers is strengthened. Indeed, such centers of attraction played important role in the several models of HTS[6–14]. Another possible experimental realization is the percolative, granular-like transition to superconductivity via hydrogen doping which has been reported in $Eu_{1.5}Ce_{0.5}NbSr_2Cu_2O_{10}$[15], a ceramic with the superconducting critical temperature T_c= 29 K.

In this paper, we shall adopt this approach and study a simple model which allows us to address the issue of superconducting transitions tuned by changing the concentration of attraction centers. Specifically, we study a two-dimensional negative U Hubbard model which has an on-site attraction on some fraction of its lattice sites and ask what fraction of sites is needed to be attractive for the system to superconduct. Recently, this issue has been addressed by Litak and Györffy [16] who examined the problem of superconducting percolation by using Hartree-Fock-Gorkov decoupling as an approximation for interacting electrons and Coherent Potential Approximation (CPA) to treat randomly distributed centers. They have found the critical concentration of negative centers $c_0 = n/2$, where n denotes a band filling in the limit of large $|U|$ interaction. For a small concentration of centers $c < c_0$ the system becomes normal because every site, where $-|U|$ interaction is present, is doubly occupied.

The effect of dilution of the interactions in the attractive U Hubbard model at half-filling, $n = 1$ can also be inferred from the Quantum Monte Carlo work of Ulmke *et al.*[17], who investigated the suppression of antiferromagnetism by $U = 0$ impurities in the repulsive Hubbard model ($U > 0$) at $n = 1$. The

critical concentration f_c of impurities which destroy the antiferromagnetism was estimated as $f_c \approx 0.45$. Since a particle-hole transformation maps the attractive and repulsive U Hubbard models onto one another, at half-filling, this work immediately identifies the critical concentration c_0 for suppression of superconductivity in the attractive Hubbard model, $c_0 = 1 - f_c = 0.55$.

Further analytic work on the disordered attractive Hubbard model, for example based on numerical solution of the Bogliubov-de Gennes equations, is contained in [18–20]. However, there have to date been no Quantum Monte Carlo (QMC) studies for the doped case where the density is not precisely half-filled and particle-hole symmetry is broken. In this paper we examine the problem of percolating superconductivity using QMC in the negative U Hamiltonian changing the concentration of negative centers c as well as band filling n[16]. The use of QMC enables us to go beyond the limitations of mean field approximations and investigate the effect of charge and pairing potential fluctuations on an equal footing.

The paper is organized as follows. After an introduction in Sec. 1 we present the microscopic model and formulate the problem (Sec. 2). Section 3 defines the QMC Monte Carlo method used in simulations and shows the key numerical results: the prediction of superconductivity percolation and the critical concentration c_0. The paper ends with conclusions.

2 The microscopic model

We consider the random negative U Hubbard Model [16] defined by the following Hamiltonian:

$$\hat{H} = -\sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{i\sigma} U_i \; c^+_{i\sigma} c_{i\sigma} c^+_{i-\sigma} c_{i-\sigma} - \mu \sum_{i\sigma} c^+_{i\sigma} c_{i\sigma} \; . \tag{1}$$

Here i and j label sites on a two-dimensional square lattice, t_{ij} is the hopping integral connecting only nearest neighbour i and j's, μ is the electronic chemical potential, $c^+_{i\sigma}$, $c_{i\sigma}$ create and annihilate, respectively, electrons at the single site i with spin σ, and the coupling constant,

$$U_i = \begin{cases} -|U| \text{ with probality } c \\ \quad 0 \text{ with probability } 1-c \end{cases} . \tag{2}$$

We are interested in determining, away from particle-hole symmetry, the critical concentration c_0 for the U centers such that for $c < c_0$ the configurationally

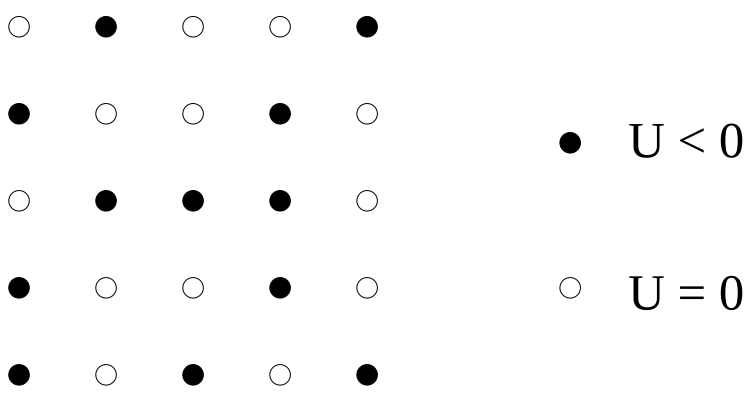

Fig. 1. The two dimensional lattice with random electron interaction $U = 0$ or $-|U|$.

averaged, superconducting long range order parameter vanishes. At the same time, we would like to obtain some insight into the mechanism of the formation of long range order as one moves to $c > c_0$.

Such questions can be addressed by computing expectation values of operators like the Hamiltonian, the kinetic energy and double occupation, and pair-pair correlation functions. Such expectation values take the general form,

$$\langle \hat{A} \rangle = \frac{\mathrm{Tr} \hat{A} \mathrm{e}^{-\beta \hat{H}}}{\mathrm{Tr} \mathrm{e}^{-\beta \hat{H}}} \ . \tag{3}$$

and can be evaluated by a standard procedure [21–24] which involves writing a path integral expression for the imaginary time evolution operator $e^{-\beta H}$ and performing a stochastic integration over a set of auxiliary fields introduced to treat the electron-electron interaction exactly. This will be described in greater detail in the following section. Typically, we can study system of a few hundred electrons, far larger than the competing exact diagonalization approach, but still small enough to require careful treatment of finite size effects, as we shall discuss below.

We will focus especially on the equal time pair correlation function, which is defined by

$$p_s(j-l) = < \Delta_l \Delta_j^+ >, \quad \text{where} \quad \Delta_j^+ = c_{j\uparrow}^+ c_{j\downarrow}^+ \tag{4}$$

Here Δ_j^+ creates a pair of electrons at lattice site i. The long range order in $p_s(l)$ can be probed by calculating its structure factor,

$$S_p = \frac{1}{N} \sum_{jl} p_s(j-l) \ . \tag{5}$$

A finite positive value $S_p > 0$, in the limit of large lattice size L, signals superconductivity, otherwise the system is normal. For our disordered system (Eq. 2, Fig. 1) we have to do a disorder average over many realizations of random configurations of the attractive U centers.

3 Details of Quantum Monte Carlo Approach

In order to describe the quantum Monte Carlo method [21] in more detail, let us first rewrite the Hubbard Hamiltonian in a way which puts the interaction term in a particle-hole symmetric form.

$$\hat{H} = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} - \sum_{i\sigma} (\mu - \frac{U_i}{2}) n_{i\sigma} + \sum_i U_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \ . \tag{6}$$

The trace over the fermion degrees of freedom cannot be performed analytically due to the quadratic interaction of term U. To reduce the problem to a quadratic Hamiltonian we discretize the imaginary time $\beta = L\Delta\tau$ (Eq. 3) and employ the Trotter approximation [25,26] to decompose the full imaginary time evolution. The partition function can be expressed as,

$$Z = Tr \mathrm{e}^{-\beta \hat{H}} = Tr \left[\mathrm{e}^{-\Delta\tau \hat{H}} \right]^L \approx \left[\mathrm{e}^{-\Delta\tau \hat{K}} \mathrm{e}^{-\Delta\tau \hat{P}} \right]^L \ , \tag{7}$$

where $\hat{K}$ includes the quadratic part of $\hat{H}$ (Eq. 6)

$$\hat{K} = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} - \sum_{i\sigma} (\mu - \frac{U_i}{2}) n_{i\sigma} \ , \tag{8}$$

while $\hat{P}$ the on-site interaction part

$$\hat{P} = \sum_i U_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \ . \tag{9}$$

Then we apply the discrete Hubbard–Stratanovich transformation to decouple the attractive interaction $U_i < 0$ [22–24]

$$e^{+\Delta\tau U_i(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})} = \frac{1}{2}e^{\frac{-|U|\Delta\tau}{4}} \sum_{Si=\pm 1} e^{\lambda S_i(n_{i\uparrow}+n_{i\downarrow}-1)} , \tag{10}$$

where

$$\cosh(\Delta\tau\lambda) = e^{\Delta\tau|U|/2} . \tag{11}$$

The replacement of the quartic interaction term between up and down spin electron densities by an expression in which the densities couple to a Hubbard-Stratonovich field makes all terms in the exponential of Eq. 7 quadratic in the fermion operators. The trace can then be performed analytically, leaving a product of determinants which depend on the Hubbard-Stratonovich field. Because the up and down spin species couple to the field with the same sign, these two determinants are identical, and hence their product is always positive. So, unlike the case of the repulsive model where $n_{i\uparrow} - n_{i\downarrow}$ couples to the field, there is no sign problem in the attractive model, even in the presence of disorder in the interaction.

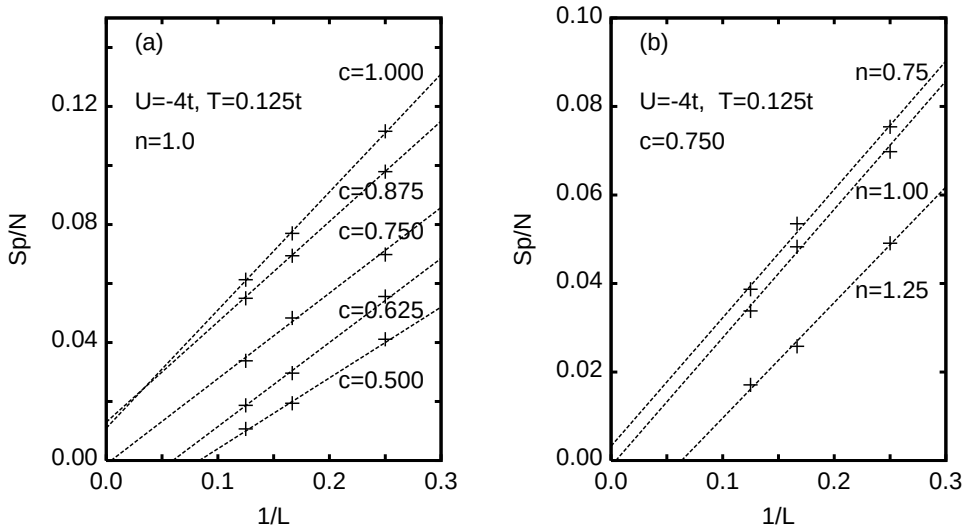

Fig. 2. Finite lattice scaling of the structure factor S_p. Each point represents the average for 20 different disordered lattice configurations (for 4×4, 6×6 and 8×8) with relatively small error.

4 Percolation of Superconductivity

Using the above procedure we have simulated the Hamiltonian (Eq. 6) and calculated the pair structure factor S_p (Eq. 5) as a function of lattice size L.

Spin-wave theory suggests that in the ordered phase the finite size correction for S_p should be proportional to the inverse linear system size $1/L$[27]. Figure 2(a) presents the results of finite size scaling of S_p for various concentrations of U sites c. The calculations were done for $U = -4t$ and $\beta = 1/T = 8/t$, and the average number of electrons per site was chosen to be $n = 1$. One can

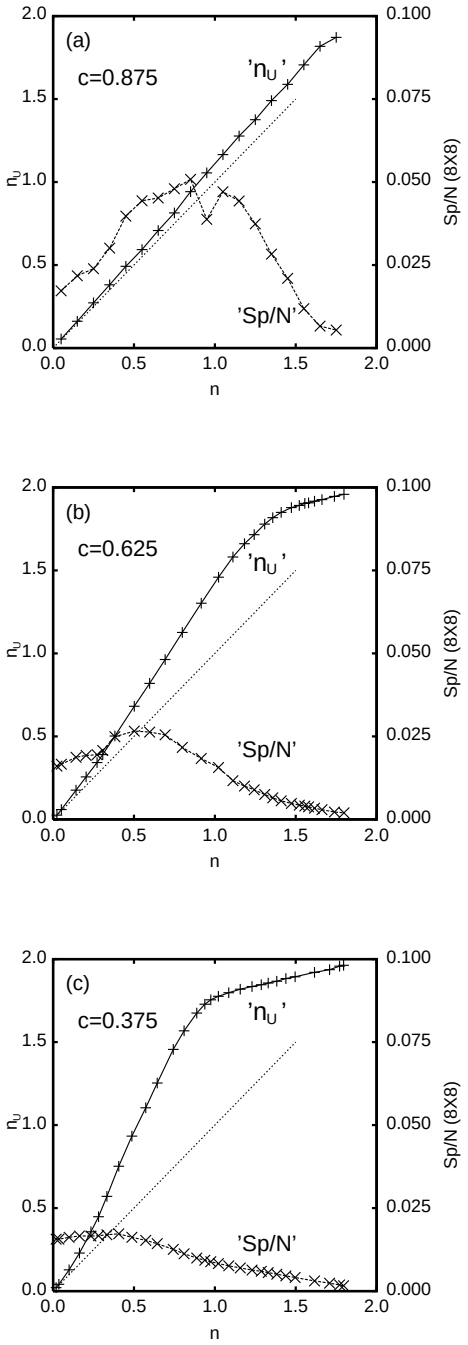

Fig. 3. Charge on U site n_U and the structure factor of pair correlation function S_p versus system filling n for a 8×8 lattice.

easily see that there exists a critical concentration $c_0 \approx 0.75$.

To see how c_0 depends on n in Fig. 2(b) the concentration of U centers is kept fixed at $c = 0.750$, and we have plotted S_p for various system fillings ($n = 0.75, 1.00$ and 1.25). Here $n = 1$ corresponds to the case at the percolation threshold ($c = c_0$). It is clear that for a larger average charge $n = 1.25$ the system is not superconducting. A different situation emerges for $n = 0.75$ where $S_p(L \to \infty)$ appears to be slightly above 0, that is, the system is superconducting. Clearly, disorder in the interaction U has broken the particle–hole symmetry. In fact, this is connected with the modification of the bare chemical potential at U sites, in the quadratic part of Hamiltonian $\hat{K}$ (Eq. 6,8)

$$\mu_{eff} = \begin{cases} \mu - U/2 & \text{for} \quad U_i = -|U| \\ \mu & \text{for} \quad U_i = 0 \end{cases} . \tag{12}$$

In some previous work on the repulsive model[17,22–24], disorder was inserted in a way which preserved particle-hole symmetry by using a separate shift in chemical potential depending on the interaction strength on each site. This enabled simulations at lower temperature since it eliminated the sign problem, but also was somewhat less physically motivated.

Interestingly, the structure factor associated with the pairing correlation function $S_p(L \to \infty)$ for $c = 1$ is smaller than the one for $c = 0.875$. This is due to the existence of a competing charge density wave (CDW) phase at $n = 1$. A similar effect was found for the system with disordered site energies and the same attraction U on every lattice site [22,28]. Thus, in addition to phase fluctuation of the pairing potential[18,19], it is clear that the distribution of charges n_i on the lattice (charge fluctuations) is also important for the destruction of superconductivity. Indeed, previous work suggests that percolation of the occupied sites is a crucial phenomenon in this process[16].

Examining this effect further, one can look for the change of the pairing factor correlation function S_p and simultaneously the average occupation of U sites (n_U) (where $U = -|U|$). Figures 3a-c show these quantities as a function of average site occupation n for a finite system 8×8 for $c = 0.875$ (a), $c = 0.625$ (b) and c=0.375 (c), respectively. Note that S_p does not display particle-hole symmetry. The dotted lines in Fig. 3(a-c) represent the occupation of attractive sites for a simplified Hamiltonian, where $\hat{K}$ reads

$$\hat{K} = -t \sum_{ij\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - \sum_{i\sigma} \mu n_{i\sigma} . \tag{13}$$

It is easy to see that in case of the full Hamiltonian (Eqs. 2,6) the system displays charge fluctuation ($n_U \neq n$) and comparing n_U curves to the dotted

lines one can see that charge fluctuations are stronger for smaller c. In our case, for large enough interaction U, the small concentration of U centers leads to double occupation in almost all attractive sites. This makes it harder for electrons to hop to another $U \neq 0$ site. Nevertheless the system can be metallic because the other electrons which occupy the $U = 0$ site can easily hop to the other $U = 0$ sites. This result is consistent with the results obtained by Litak and Györffy [16]. The small dip visible in the pairing structure factor S_p around $n = 1$ (in Fig. 3a) can be associated with the creation of a CDW order. This effect is not present in Figs. 3b-c as CDW expected to disappear faster than superconductivity [22,28].

5 Conclusions

We have examined the problem of percolating superconductivity in the context of a random U Hubbard model. We have studied the case where U_i is $-|U|$ and 0 with probability c and $1 - c$ respectively by the quantum Monte Carlo method. For the half–filled system $n = 1$ we obtain the critical concentration $c_0 = 0.75$. As we expected the transition is due to phase and charge fluctuations and depends strongly on the density n. In that sense our results agree qualitatively with those obtained by Litak and Györffy[16]. Moreover, the present approach is exact as opposed to earlier work[16] employing the mean field approximation. We find that the onset of superconductivity in this diluted, attractive Hubbard model is linked to percolation of the order parameter and charge fluctuations.

Acknowledgements

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